The Nanoscience Cooperative Research Center, CIC nanoGUNE, located in Donostia / San Sebastian, Basque Country (Spain), is currently looking for a

MASTER STUDENT

to work on

QUANTUM COMPUTING FOR FIRST-PRINCIPLES CALCULATIONS OF CORRELATED ELECTRONS

NanoGUNE is a research center devoted to conducting world-class nanoscience research for a competitive growth of the Basque Country. NanoGUNE is a member of the Basque Research and Technology Alliance (BRTA) and is recognized by the Spanish Research Agency as a *María de Maeztu* Unit of Excellence.

The solution of quantum many-particle systems is one of the most natural problems to be addressed with quantum computing, since the exponential growth of the system's Hilbert space with the size of the system is matched by the exponential growth of the space associated with growing numbers of entangled qubits. In a collaboration between the Theory group at Nanogune and IBM Quantum at Zurich we are working on the connection of a large-scale first-principles method for addressing weakly correlated systems from first principles on conventional supercomputers (SIESTA) with a program running on quantum computers (IBM's QISKIT) that can address the (nearly) exact solution of the correlated system given by an active space embedded into a larger, less correlated one. For a first proof of concept, quantum eigensolver methods will be used on IBM's quantum computers to obtain correlated solutions for the complete active space spanned by the relevant orbitals of a few atoms (e.g. a transition-metal ion substitution) in a material that can be otherwise sensibly treated using density-functional theory, which is a widely used mean-field-like method for first-principles calculations. The student will engage in the development, testing, and first applications of the software, using supercomputers linked to IBM's quantum computers.

The **position** is offered in the **Theory Group**, led by **Emilio Artacho** (e.artacho@nanogune.eu). More information can be found at https://www.nanogune.eu/en/research.

The position is expected to start in **01/09/2025** and for a total length of **up to 10 months** (01/09/2025 - 30/06/2026).

Candidates should **apply** by completing the **form below** and attaching the following documents:

a. A complete CV
b. Academic Record and Cover Letter grouped in a single PDF file

The **deadline** for applications is **22/06/2025**.

NOTES:
(i) All applicants will receive an answer after the end of the selection process; but please note that due to the large number of submissions that are expected, we cannot provide individual feedback.
(ii) Additional information about nanoGUNE's commitment towards HR excellence in Research and Gender Equality are available on our website.
(iii) We encourage you to subscribe to our HR mailing list to receive information related to nanoGUNE's open positions and open calls for different training and talent attraction programs.

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